

Grain Boundary Engineering

Scientific Achievement

By employing epitaxial templating techniques developed at Argonne National Laboratory thin-film materials with controlled interfacial geometries have been produced. Control of grain boundary (GB) geometry is of importance when designing favorable materials properties and when specific grain orientations are required for atomic-level studies of GB structure. Whereas conventional high-resolution electron microscopy (HREM) is limited to tilt GBs, atomic-level GB structure investigations have been possible for general and twist GBs using the epitaxial templating technique. The latter also allows direct comparisons of GB structure between different materials, such as Au, Al, MgO. Control of in-plane grain geometry is also possible. In this manner GB arrays can be formed for studies in GB migration and possible applications for electrical and thermal transport of GBs.

High-purity Au films are epitaxially grown by UHV electron-beam evaporation on (110) or (001) NaCl single crystalline substrates. To produce tilt grain boundaries (110) or (001) Au films are placed on (110) or (001) NaCl substrates respectively at the desired in-plane misorientation. The Au film is removed completely in certain areas by low-energy Ar sputtering through a physical mask while in the remaining areas only a thin seed layer of Au is retained. The NaCl substrate prepared in this manner is then the template for production of a mazed tilt bicrystal by UHV e-beam evaporation of Au. MgO films grown on such (110) Au films can exactly replicate the underlying grain structure. Other types of oxides, such as NiO can be grown when assisted by an oxygen plasma. Subsequently other materials such as Al can be grown epitaxially, again replicating the underlying grain structure. When a (110) film is placed on a (001) substrate or vice versa, the results are side by side (001) and (110) grains. This configuration has been used to produce twist and general GBs in Au. In this manner it has been possible for the first time to systematically study the atomic-scale structure of twist and general grain boundaries by HREM. Comparison of the atomic-scale structure of GBs in Au and Al have revealed dramatic differences when the interatomic interactions favor the formation of stacking faults and twins in Au, but not in Al which has a much higher stacking fault energy.

Significance

The properties of interfacial materials depend on interfacial composition, geometry and atomic-scale structure. Therefore, the control of these factors are of great importance in designing useful materials. The present study allowed the control of GB geometry which opened up a new range of experimental studies concerning the atomic-scale structure of GBs. In addition, epitaxial GB templating techniques may find applications in high-technology devices, such as varistors and high-Tc SQUIDS.

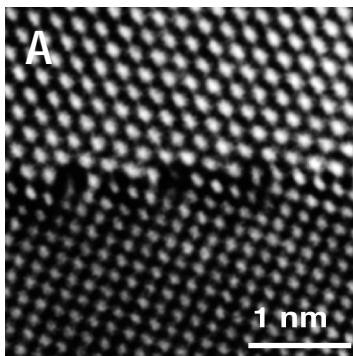
Performers:

K. L. Merkle and L. J. Thompson, Phys. Rev. Lett. **83**, 556 (1999)).

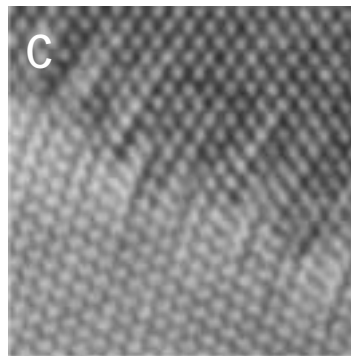
K. L. Merkle, L. J. Thompson, F. Phillipp (MPI Stuttgart) Phys. Rev. Lett. **88**, 225501 (2002).

K. L. Merkle, Electron Microscopy: Its Role in Materials Science (The Mike Meshii Symposium) TMS 2003, p. 33-42.

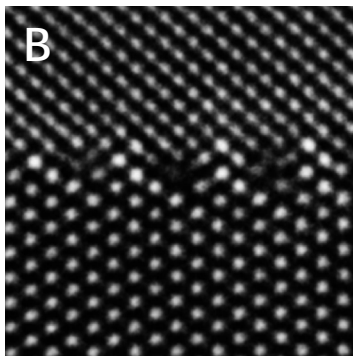
Grain Boundary Engineering



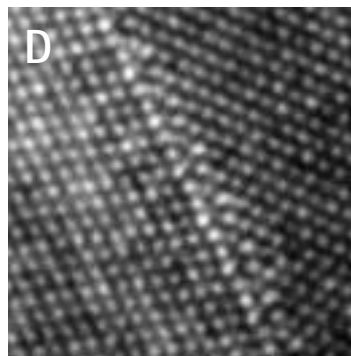
Au general GB



MgO [110] tilt GB



Au twist GB



Al [110] tilt GB

Epitaxial templating techniques are used to control grain boundary (GB) crystallography.

High-resolution electron micrographs of A) general GB in Au, B) a microfaceted twist GB in Au, C) an MgO, [110] tilt GB templated onto a gold bicrystal of the same geometry, and D) an Al GB templated onto MgO.

Seed crystals of Au on NaCl substrates are used to produce bicrystals of specific geometries used to study the atomic structure of GBs in different materials.

The control of GB geometries is of key importance for understanding GB structure and obtaining desirable GB function.

K. L. Merkle, L. J. Thompson